Synthesis and Characterization of 6-((2-(pyridin-2-yl)hydrazono)methyl)–pyridin-2-yl)methanol: Supramolecular and Topological Study.

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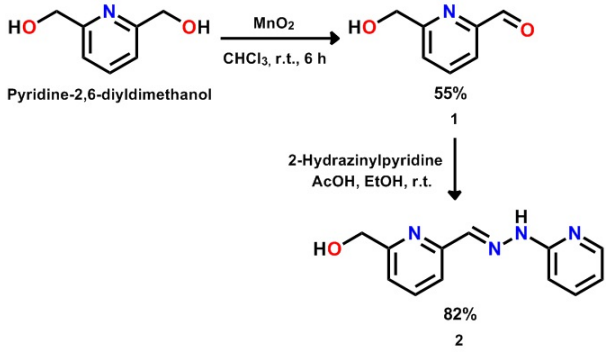
Abstract

6-((2-(pyridin-2-yl)hydrazono)methyl)pyridin-2-yl)methanol was synthetized with 82% yield, crystalized in the monoclinic space group C 2/c and presents a configuration *E* with respect to the C7=N2 bond hydrazone framework. Crystal packing is formed by N—H···N, O—H···N and C—H···C interactions. These interactions give rise to layers in the plane (121). The layers are stacking along [10-2] to obtain the 3D supramolecular structure. The intermolecular interactions were analyzed by the Hirshfeld surface and the 2D supramolecular arrangement was topologically simplified as a **hcb** network.



1. Introduction

Hydrazones are imine type compounds with the R^1R^2**C=N—N**R^3R^4 framework. Depending on the nature of the R substituents these compounds exhibit a very versatile chemistry. In general, hydrazones have caught the attention for their potential use as molecular systems, capable of undergoing reversible changes of configuration, *E/Z* isomerization, (Su and Aprahamian, 2014; Tatum *et al.*, 2014). These compounds may exhibit coordination dynamics by the presence of coordination sites in the chemical structure (Ghosh *et al.*, 2011), this feature allows the locking and unlocking, controlled by metal ions, and therefore the reversible transformation of different states (Chaur *et al.*, 2011). Properties that are suitable for dynamic combinatorial chemistry (DCC).

The aforementioned properties of hydrazones have enabled them to be use in supramolecular chemistry (Su and Aprahamian, 2014), as molecular switches (Cnossen *et al.*, 2014; Yamamura *et al.*, 1992), metallo-assemblies (Lehn and Ulrich, 2009; Ruben *et al.*, 2006; Hardy, 2013) and sensors (Su and Aprahamian, 2014; Tatum *et al.*, 2014) of both cations and anions. Likewise other systems including light driven molecular motors have been developed (Cnossen *et al.*, 2014) and in that sense many of these systems can be implemented as digital molecular information storage systems due to the multiple dynamics that they exhibit in a reversible fashion.

A search in the CCDC database (Groom and Allen, 2014) reveal that hydrazones derived from the 6-((2-(pyridin-2-yl)hydrazono)methyl)pyridine are used in the synthesis of several complexes (79 hits). The presence of at least three coordinatively active N positions and the posibility to functionalize the aromatic rings makes to this a very interesting template. Compounds with divalent transition metals as Cu^{2+}, Zn^{2+}, Co^{2+}, Ni^{2+} and Ru^{2+} (Ghosh *et al.*, 2011; Rojo *et al.*, 1988; Chaur *et al.*, 2011; Ghosh *et al.*, 2013; Chiumia *et al.*, 1999; Stadler *et al.*, 2010) are observed. Also, these kind of derivates are found coordinate to metals as Pb^{2+}, Yb^{3+}, Hg^{2+} and Mo^{0} (Ulrich *et al.*, 2009; Baraniak *et al.*, 1976; Ulrich & Lehn, 2009; Bruce *et al.*, 1974). The crystallographic data of few organics compounds derived from the 2-hydrazinopyridine are reported (13 hits). The compound reported by Ulrich *et al.*, 2009, named (E)-(2-(2-((4-((((dimethyl(t-butyl)-silyl)oxy)methyl)-2-pyridinyl)methylene) hydrazino)-4-pyridinyl)methanol is the most similar with a crystal packing formed by O—H···N and N—H···N interactions.

Our group has paid special interest in those hydrazones derived from the 2-pyridinecarboxaldehyde and 2-hydrazinepyridine since these type of compound exhibit the well-known reversible photoinduced *E/Z* isomerization, coordination to metal centers and they possesses an acidic N—H proton. The latter allows the formation of intramolecular hydrogen bonds adding special properties and new supramolecular architectures. Herein we report the synthesis, crystallographic characterization, topology and Hirshfeld surface calculation of the hydrazone 6-((2-(pyridin-2-yl)hydrazono)methyl)-pyridin-2-yl)methanol a potential molecule to be use in dynamic supramolecular chemistry.

2. Experimental

The title compound was prepared by the condensation reaction between the aldehyde 1 and the 2-hydrazinopyridine in ethanol resulting in a yellow solid with 82% yield (see scheme 1).

2.1. Synthesis and crystallization

The title compound was prepared by the condensation reaction between the aldehyde **1** and the 2-hydrazinopyridine in ethanol resulting in a yellow solid with 82% yield (see scheme 1).

6-(hydroxymethyl)picolinaldehyde (1): A solution of pyridine-2,6-diyldimethanol (140 mg, 1 mmol) in chloroform (5 mL) was stirred with manganese dioxide (440 mg, 5 mmol) at room temperature for 6 hours. Then, the reaction mixture was filtered through Celite and the solvent was removed by evaporation to get a yellow oil which was purified by column chromatography using silica gel as stationary phase and a mixture of chloroform/methanol 9/1 as eluent to get the desired product as a colorless oil (55% yield). ^{1}H NMR (DMSO-d_6, 400 MHz) δ/ppm = 9.94 (s, 1H), 8.06 (t, J = 7.7 Hz, 1H), 7.82 (d, J = 7.5 Hz, 1H), 7.79 (d, J = 7.8 Hz, 1H), 5.67 (t, J = 5.7 Hz, 1H), 4.69 (d, J = 5.6 Hz, 2H). ^{13}C NMR (DMSO-d_6, 100 MHz) δ/ppm = 194.19, 163.38, 151.88, 138.66, 125.41, 120.53, 64.37.

6-((2-(pyridin-2-yl)hydrazono)methyl)pyridin-2-yl)methanol (2): A solution of 2-hydrazinopyridine (110 mg, 1 mmol) in ethanol (1 ml) was added to a solution of **1** (138 mg, 1 mmol) in ethanol (1 ml) containing a catalytic amount of acetic acid. The resulting precipitate was washed several times with small portions of cold chloroform and then it was recrystallized from absolute ethanol to afford yellow needles (m.p. 190.2- 191.0°C, 82% yield). ^{1}H NMR (DMSO-d_6, 400 MHz) δ/ppm = 11.13 (s, 1H), 8.13 (d, *J* = 4.9 Hz, 1H), 8.03 (s, 1H), 7.84-7.77 (m, 2H), 7.66 (t, *J* = 7.8 Hz, 1H), 7.37 (d, *J* = 8.4, 1H), 7.29 (d, *J* = 7.8 Hz, 1H), 6.83 – 6.78 (m, 1H), 5.41 (t, *J* = 5.9 Hz, 1H), 4.56 (d, *J* = 5.8 Hz, 2H). ^{13}C NMR (DMSO-d_6, 100 MHz) δ/ppm = 162.07, 157.18, 153.78, 148.32, 139.78, 138.55, 137.45, 119.75, 117.47, 116.05, 107.04, 64.63. FT—IR (KBr) /cm^{-1} = 3421 (O—H), 3201 (N—H), 2924 y 2851 (C—H), 1602 (C=C) 1578 (C=N), 1090 (C—O). MS (EI, 70 eV) *m/z* (%): 228 (M^{+}, 13). Anal. Calcd for $C_{12}H_{12}N_4O$: C 63.15, H 5.30, N 24.55%; Found: C 62.77, H 5.38, N 24.32%.

2.2. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. All H atoms bonded to C atoms were placed in idealized positions, with C—H bond lengths fixed to 0.93 (aromatic C—H) or 0.97 Å (methylene). H atoms bonded to N and O atoms were found from the Fourier map. The N—H and O—H distances were 0.96 and 0.94 Å respectively. All calculated H atoms were refined as riding with displacement parameters calculated as Uiso(H) = xUeq(carrier C) where x = 1.2.

3. Results and discussion

The molecular structure of the title compound is illustrated in the Fig. 1. This compound crystalized in the monoclinic space group C 2/c and present a configuration *E* with respect to the C7=N2 bond of the hydrazone framework. The two pyridinic rings present a torsion angle of -171.33 (15)° and 176.72 (14)° for N1–C5–C7–N2 and N4–C8–N3–N2 respectively.

The crystal packing is formed via hydrogen bonds. The two self-complementary N3—H3···N4 interaction with a distance of 3.045 (2) Å give rise to dimers to generate the $R^2_2(8)$ homosynthon Fig. 2. The dimers are connected each other by top-tail O1–H1···N1 interactions with a distance of 2.912 (2) Å Fig. 2. This conformation allows the join of dimeric subunits along [111] and [010] directions giving rise to layers in the plane (121). Weak interactions join the layers stacking along to [10-2] direction Fig.3. The intermolecular interaction distances and angles are summarized in table 1.

The 2D supramolecular arrangement was topologically simplified. Each molecule is interconnected by hydrogen bonds acting as 3- connected nodes. This connectivity give rise to 2D network type **hcb** (Shubnikov hexagonal plane net/(6,3)) (Figure 4) with point symbol (6^3) (Blatov *et al.*, 2014).

The analysis of the Hirshfeld surface supports the information present in the supramolecular and topological analysis. This surface shows the susceptible areas to strong and weak contacts. It can be identify in the color pattern on the surface as concave red curvature for the acceptor region around to N and O atoms with free electron pairs (Figure 5, a) and b)). The convex blue curvature for the donor groups is observed mainly in the N—H, O—H and C—H region (McKinnon *et al.*, 2004; Hirshfeld, 1977). The finger prints graphic (Figure 6) present a symmetric behavior where the two sharp peaks projecting towards the bottom of the fingerprint plot is due to strong N—H···N interactions (acceptor: lower peak $d_e<d_i$) and O—H···N (Donor: top peak $d_e>d_i$) (Spackman and McKinnon, 2002). The most important interaction can be evaluated by overlapping contributions from the hydrogen interactions which includes N···H, H···N, H···H, O···H and C···H (Figure 6). This analysis show that the H···H and C···H interactions contribute in largest value to the Hirshfeld surface with 44.7% and 14.3% respectively. The N···H interactions that corresponding with the homosynthon formation contribute with 10.1%, while the H···N interaction that involve the dimmers conectivity and other interactions contribute with 7.4%. Finally, the strong O···H interaction contribute with the 3.5% of the surface.

In conclusion, we have synthetized and structurally characterized the novel compound (E)-6-((2-(pyridin-2-yl)hydrazono)methyl)pyridin-2-yl)methanol. The crystal structure presents weak intermolecular interactions, as well as hydrogen bonds, forming homosynthon subunits that build a 2D arrangement. The molecule was topologically simplified as 2D network type **hcb.** Hirshfeld surface analysis support the importance of N···H intermolecular interactions as responsible for the formation of the 2D arrangement. Also reveal that the weak H···H and C···H interaction are involved in the stacking of the layers giving rise to 3D molecular close packing. Synthesized hydrazone molecule is able to be coordinated to metal centers and therefore it have potential use in supramolecular dynamic systems, molecular machines and information storage devices.

Table 1

Hydrogen-bond geometry (Å, º) for 6-((2-(pyridin-2-yl)hydrazono)methyl)pyridin-2-yl)methanol

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N3—H3*A*···N4^{i}	0.96 (2)	2.08 (2)	3.045 (2)	180 (2)
O1—H1···N1^{ii}	0.94 (2)	1.98 (3)	2.912 (2)	170 (2)

Symmetry codes: (i) −*x*, −*y*+1, −*z*+1; (ii) −*x*+1/2, *y*−1/2, −*z*+3/2.

Table 2

Experimental details

Crystal data	
Chemical formula	$C_{12}H_{12}N_4O$
M_r	228.26
Crystal system, space group	Monoclinic, *C*2/*c*
Temperature (K)	291
a, *b*, *c* (Å)	23.461 (5), 5.5965 (13), 17.068 (3)
β (°)	96.544 (13)
V (Å^3)	2226.4 (8)
Z	8
Radiation type	Mo *K*α
μ (mm^{-1})	0.09
Crystal size (mm)	0.2 × 0.1 × 0.05
Data collection	
Diffractometer	KappaCCD diffractometer
Absorption correction	–
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	21975, 2255, 1116
R_{int}	0.134
$(\sin \theta/\lambda)_{max}$ (Å^{-1})	0.624
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.043, 0.109, 0.83
No. of reflections	2250
No. of parameters	156
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.16, −0.14

Computer programs: Collect (Nonius, 1998), *HKL SCALEPACK* (Otwinowski & Minor 1997), *HKL DENZO* and *SCALEPACK* (Otwinowski & Minor 1997), *SHELXS2013* (Sheldrick, 2015), *SHELXL2014*/7 (Sheldrick, 2015), *ORTEP* for Windows (Farrugia, 2012), *Mercury* (Macrae *et al.*, 2008), TOPOS (Blatov *et al.*, 2014) and CrystalExplorer (McKinnon *et al.*, 2004), *WinGX* publication routines (Farrugia, 2012).

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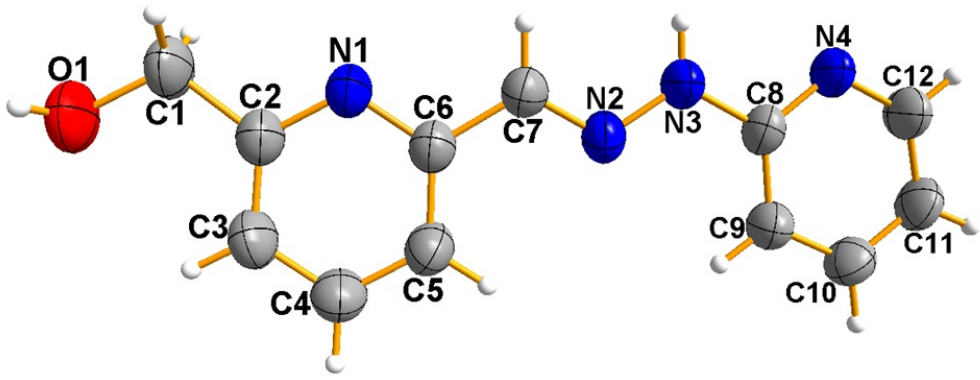

Figure 1

ORTEP representation of the title compound, showing the atom labelling. Displacement ellipsoids are drawn at the 50% probability level.

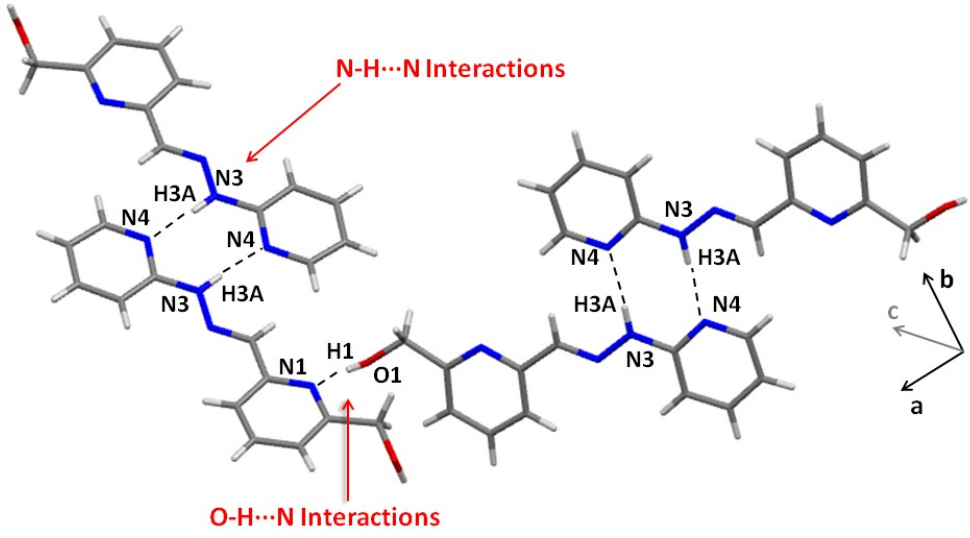

Figure 2

Representacion of the dimers formed by N-H···N (i) interactions and the O-H···N (ii) interdimer interactions. Symmetry code: (i) -x,-y+1,-z+1 and (ii) -x+1/2,y-1/2,-z+3/2.

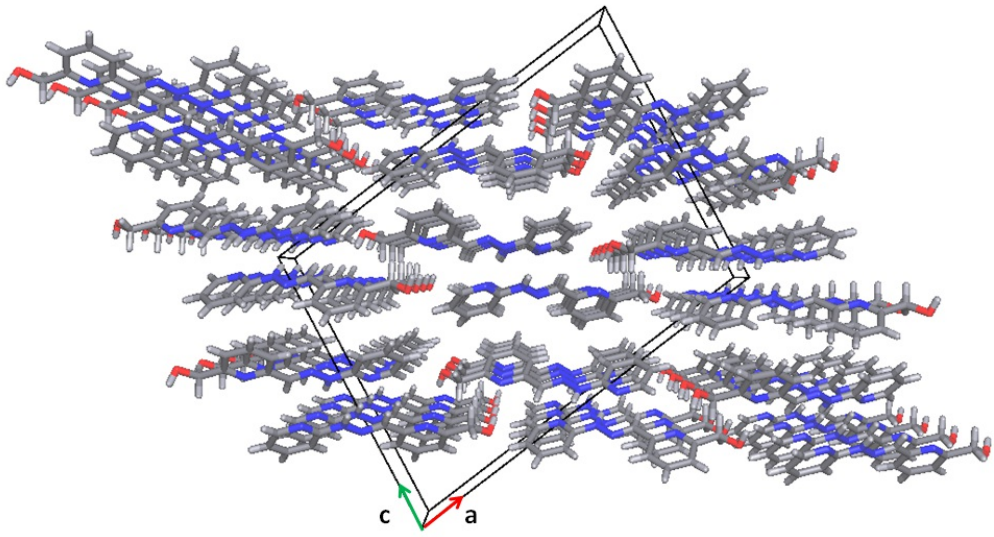

Figure 3

Crystal packing representation of the title compound view along [10-2] direction.

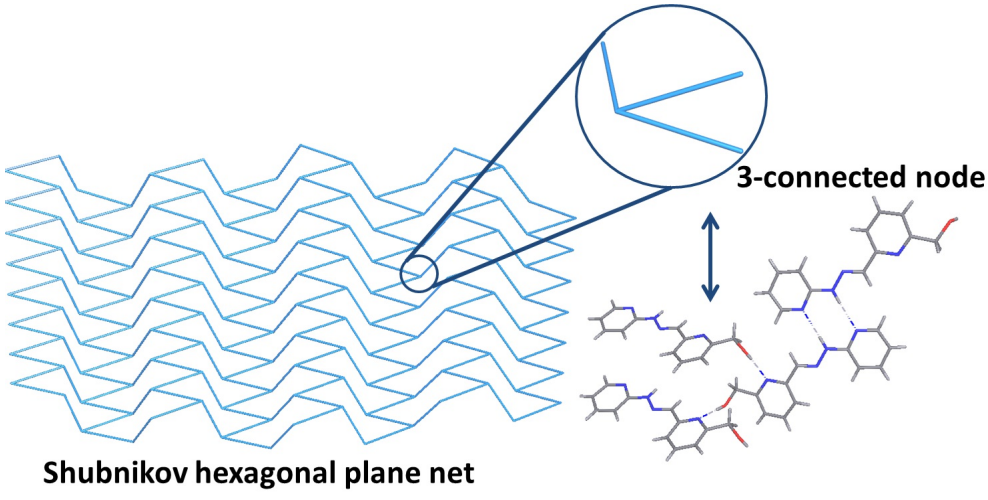

Figure 4

Topological simplification of 6-((2-(pyridin-2-yl)hydrazono)methyl)pyridin-2-yl)methanol compund.

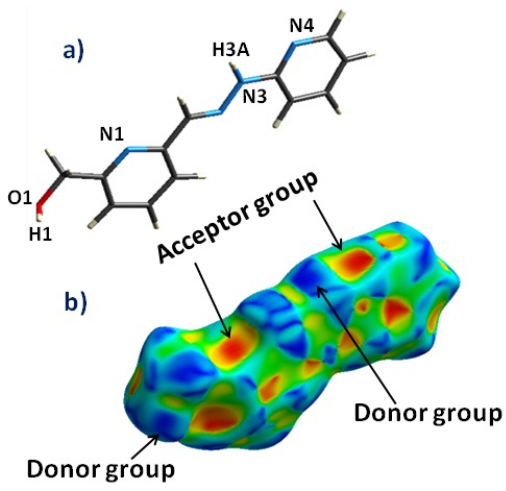

Figure 5

a) Molecular representation in the same orientation of the b) Hirshfeld surface.

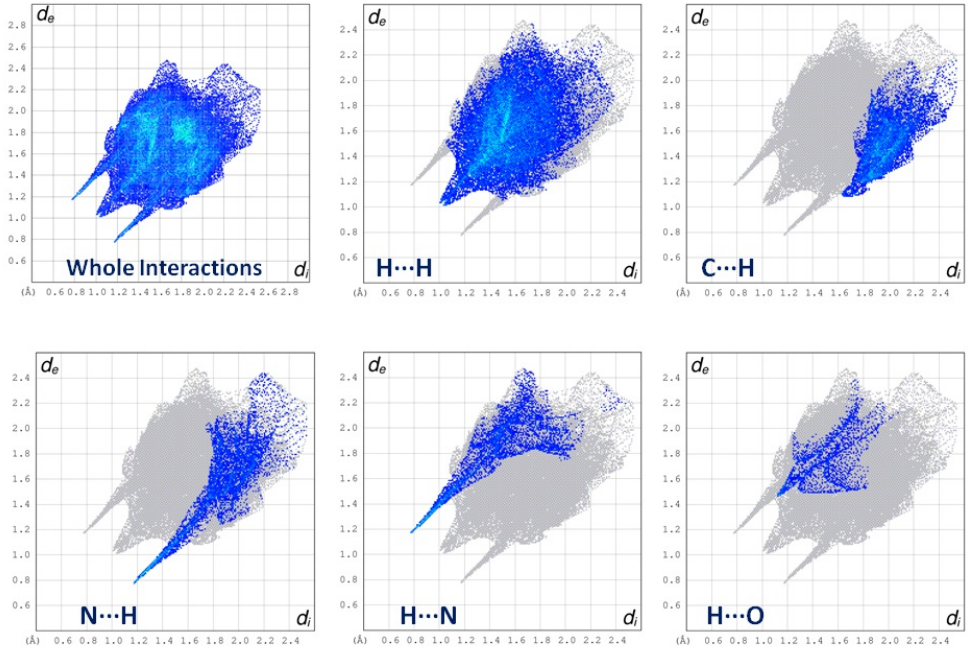

Figure 6

Bidimensional fingerprint plot for whole molecule and H···H, C···H, N···H, H···N, H···O close contacts.

supporting information

Synthesis and Characterization of 6-((2-(pyridin-2-yl)hydrazono)methyl)–pyridin-2-yl)methanol: Supramolecular and Topological Study.

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Computing details

Data collection: Collect (Nonius, 1998); cell refinement: *HKL SCALEPACK* (Otwinowski & Minor 1997); data reduction: *HKL DENZO* and *SCALEPACK* (Otwinowski & Minor 1997); program(s) used to solve structure: *SHELXS2013* (Sheldrick, 2015); program(s) used to refine structure: *SHELXL2014*/7 (Sheldrick, 2015); molecular graphics: *ORTEP* for Windows (Farrugia, 2012), *Mercury* (Macrae *et al.*, 2008), TOPOS (Blatov *et al.*, 2014) and CrystalExplorer (McKinnon *et al.*, 2004); software used to prepare material for publication: *WinGX* publication routines (Farrugia, 2012).

'6-((2-(pyridin-2-yl)hydrazono)methyl)pyridin-2-yl)methanol'

Crystal data

$C_{12}H_{12}N_4O$
$M_r = 228.26$
Monoclinic, $C2/c$
$a = 23.461\ (5)$ Å
$b = 5.5965\ (13)$ Å
$c = 17.068\ (3)$ Å
$\beta = 96.544\ (13)°$
$V = 2226.4\ (8)$ Å^3
$Z = 8$
$F(000) = 960$
$D_x = 1.362$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 2000 reflections
$\theta = 2.9–26.4°$
$\mu = 0.09$ mm^{-1}
$T = 291$ K
Neddle, yellow
0.2 × 0.1 × 0.05 mm

Data collection

KappaCCD diffractometer
21975 measured reflections
2255 independent reflections
1116 reflections with $I > 2\sigma(I)$
$R_{int} = 0.134$
$\theta_{max} = 26.4°$, $\theta_{min} = 3.1°$
$h = -28\rightarrow28$
$k = -6\rightarrow6$
$l = -21\rightarrow21$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.043$
$wR(F^2) = 0.109$
$S = 0.83$
2250 reflections
156 parameters
0 restraints
Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0585P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.16$ e Å^{-3}
$\Delta\rho_{min} = -0.14$ e Å^{-3}

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	0.24078 (7)	−0.1570 (3)	0.81410 (11)	0.0639 (5)
H1A	0.2627	−0.1388	0.7696	0.077*
H1B	0.2406	−0.0037	0.8406	0.077*
C2	0.17994 (7)	−0.2219 (3)	0.78368 (10)	0.0517 (5)
C3	0.15197 (7)	−0.4185 (3)	0.80988 (11)	0.0578 (5)
H3	0.1703	−0.5176	0.8487	0.069*
C4	0.09660 (7)	−0.4656 (3)	0.77769 (11)	0.0595 (5)
H4	0.0773	−0.5990	0.7937	0.071*
C5	0.07007 (7)	−0.3131 (3)	0.72164 (11)	0.0567 (5)
H5	0.0328	−0.3425	0.6990	0.068*
C6	0.09996 (7)	−0.1148 (3)	0.69958 (10)	0.0497 (4)
C7	0.07409 (7)	0.0627 (3)	0.64367 (10)	0.0534 (5)
H7	0.0968	0.1816	0.6253	0.057 (5)*
C8	−0.05915 (7)	0.2219 (3)	0.54167 (10)	0.0503 (4)
C9	−0.09482 (7)	0.0371 (3)	0.55988 (10)	0.0566 (5)
H9	−0.0808	−0.0876	0.5926	0.068*
C10	−0.15108 (7)	0.0433 (3)	0.52850 (11)	0.0610 (5)
H10	−0.1758	−0.0798	0.5388	0.073*
C11	−0.17111 (8)	0.2337 (3)	0.48139 (11)	0.0611 (5)
H11	−0.2093	0.2424	0.4600	0.073*
C12	−0.13305 (7)	0.4076 (3)	0.46750 (11)	0.0592 (5)
H12	−0.1466	0.5356	0.4360	0.071*
N1	0.15471 (5)	−0.0724 (2)	0.72889 (8)	0.0509 (4)
N2	0.02035 (6)	0.0560 (2)	0.61977 (8)	0.0552 (4)
N3	−0.00141 (6)	0.2294 (3)	0.57003 (9)	0.0588 (4)
N4	−0.07727 (6)	0.4078 (2)	0.49593 (9)	0.0549 (4)
O1	0.26852 (6)	−0.3248 (2)	0.86646 (8)	0.0732 (4)
H1	0.2962 (11)	−0.408 (4)	0.8416 (16)	0.132 (10)*
H3A	0.0234 (8)	0.344 (3)	0.5493 (12)	0.086 (6)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0537 (11)	0.0719 (11)	0.0624 (13)	0.0080 (9)	−0.0088 (10)	0.0061 (10)
C2	0.0470 (10)	0.0599 (10)	0.0476 (11)	0.0083 (8)	0.0030 (8)	0.0006 (9)
C3	0.0565 (11)	0.0645 (11)	0.0518 (12)	0.0101 (9)	0.0042 (9)	0.0079 (9)
C4	0.0580 (12)	0.0625 (11)	0.0588 (13)	−0.0022 (9)	0.0104 (10)	0.0066 (9)
C5	0.0452 (10)	0.0659 (10)	0.0585 (12)	−0.0014 (8)	0.0033 (9)	0.0049 (10)
C6	0.0452 (10)	0.0567 (10)	0.0463 (11)	0.0032 (8)	0.0017 (8)	0.0009 (8)
C7	0.0479 (11)	0.0598 (10)	0.0513 (12)	−0.0030 (9)	0.0000 (9)	0.0052 (9)
C8	0.0441 (10)	0.0574 (10)	0.0479 (11)	0.0000 (8)	−0.0020 (8)	−0.0026 (9)
C9	0.0520 (11)	0.0597 (10)	0.0567 (12)	−0.0045 (8)	0.0001 (9)	0.0075 (9)
C10	0.0527 (11)	0.0697 (12)	0.0605 (13)	−0.0119 (9)	0.0066 (10)	−0.0004 (10)
C11	0.0420 (10)	0.0782 (12)	0.0611 (13)	−0.0021 (9)	−0.0029 (9)	−0.0008 (10)
C12	0.0489 (11)	0.0639 (11)	0.0627 (13)	0.0042 (9)	−0.0030 (9)	0.0074 (9)
N1	0.0442 (8)	0.0572 (8)	0.0499 (9)	0.0037 (6)	−0.0007 (7)	0.0018 (7)
N2	0.0474 (9)	0.0630 (9)	0.0530 (10)	0.0025 (7)	−0.0031 (7)	0.0066 (7)
N3	0.0456 (9)	0.0620 (9)	0.0657 (11)	−0.0005 (7)	−0.0073 (8)	0.0155 (8)

N4	0.0466 (8)	0.0572 (8)	0.0584 (10)	0.0009 (7)	−0.0053 (7)	0.0069 (7)
O1	0.0615 (9)	0.0894 (9)	0.0648 (10)	0.0171 (7)	−0.0100 (7)	0.0092 (8)

Geometric parameters (Å, º) for 6-((2-(pyridin-2-yl)hydrazono)methyl)pyridin-2-yl)methanol

C1—O1	1.4043 (19)	C7—N2	1.2808 (19)
C1—C2	1.507 (2)	C8—N4	1.3407 (19)
C2—N1	1.341 (2)	C8—N3	1.386 (2)
C2—C3	1.381 (2)	C8—C9	1.387 (2)
C3—C4	1.377 (2)	C9—C10	1.367 (2)
C4—C5	1.376 (2)	C10—C11	1.384 (2)
C5—C6	1.388 (2)	C11—C12	1.360 (2)
C6—N1	1.3454 (19)	C12—N4	1.343 (2)
C6—C7	1.461 (2)	N2—N3	1.3508 (18)
O1—C1—C2	114.21 (15)	N4—C8—N3	114.34 (14)
N1—C2—C3	122.31 (15)	N4—C8—C9	123.33 (15)
N1—C2—C1	114.53 (15)	N3—C8—C9	122.33 (15)
C3—C2—C1	123.15 (15)	C10—C9—C8	118.25 (16)
C4—C3—C2	118.97 (16)	C9—C10—C11	119.71 (16)
C5—C4—C3	119.36 (16)	C12—C11—C10	117.78 (16)
C4—C5—C6	118.79 (16)	N4—C12—C11	124.74 (16)
N1—C6—C5	122.07 (15)	C2—N1—C6	118.41 (14)
N1—C6—C7	115.52 (14)	C7—N2—N3	117.84 (14)
C5—C6—C7	122.41 (15)	N2—N3—C8	118.81 (15)
N2—C7—C6	120.58 (16)	C8—N4—C12	116.17 (14)

Hydrogen-bond geometry (Å, º) for 6-((2-(pyridin-2-yl)hydrazono)methyl)pyridin-2-yl)methanol

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N3—H3*A*···N4^{i}	0.96 (2)	2.08 (2)	3.045 (2)	180 (2)
O1—H1···N1^{ii}	0.94 (2)	1.98 (3)	2.912 (2)	170 (2)

Symmetry codes: (i) −*x*, −*y*+1, −*z*+1; (ii) −*x*+1/2, *y*−1/2, −*z*+3/2.